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MERCURY vs. TART Comparisons to Verify Thermal Scattering

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DISCLAIMER

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Introduction

We have verified that MERCURY [1] can accurately model both free atom and bound atom neutron thermal scattering. This was accomplished by comparing MERCURY and TART [2] results, for a series of reactor pin-cells, that were earlier calculated by a number of Monte Carlo transport codes [3]. For decades TART has been compared to other codes and found to be in excellent agreement. In particular, in this earlier study [3], TART performed very well compared to these other codes, and TART is here used as a standard to which MERCURY results are compared.

Compared to the spread in the results found in the earlier study [3], here the agreement between MERCURY and TART results are incredible. Even for simple scalar integral parameters, such as K-eff, in this earlier study differences of up to over 2% were found. Here the differences in K-eff between MERCURY and TART results are closer to 0.01%, two decades smaller than the differences seen in the earlier study [3].

Here we present the results of our MERCURY vs. TART comparisons and we also explain how we were able to obtain such incredible agreement. Lastly we illustrate the importance of using thermal scattering law data.

Overview

Recently the results from many Monte Carlo codes were compared for a series of theoretical pin-cells; the results are documented in ref. [3]; details are also provided here in Appendix A and B. The purpose of this earlier code comparison was primarily to determine how accurately our codes model both bound and free atom neutron thermal scattering. Prior to this study many people assumed that our Monte Carlo transport codes were all now so accurate that they would all produce more or less the same answers, say for example K-eff to within 0.1%. The results demonstrated that in reality we see a rather large spread in the results for even simple scalar parameters, such as K-eff, where we found differences in excess of 2%, far exceeding many people's expectations.

The differences between code results were traced to four major factors,

1) Differences between the sets of nuclear data used.
2) The accuracy of nuclear data processing codes.
3) The accuracy of the models used in our Monte Carlo transport codes.
4) Code user selected input options.

Naturally at Livermore we would like to insure that we minimize the effects of these factors. In this report we compare the results using two of our Monte Carlo transport codes: MERCURY {2] and TART [2], with the following constraints designed to address the four points listed above,

1) Both codes used exactly the same nuclear data, namely the TART 2005 data.
2) Each code used its own nuclear data processing code. Even though these two data processing codes are independent, they have been extensively tested to insure the processed output results closely agree.
3) Both used the same nuclear physics models. This required that some physics be turned off in each code, namely,
    a) Unresolved resonance energy region self-shielding was turned off in TART, since this is not currently available in MERCURY.
    b) Delayed neutrons were treated as prompt in TART, since this is not currently available in MERCURY.
    c) Classical, rather than relativistic, kinematics were used in MERCURY, since relativistic kinematics is not currently available in TART.
4) Both codes used the same input options; both modeled the geometry and materials in exactly the same manner; both used the same number of neutron histories to produce results to within comparable statistical accuracy.

These constraints were used to test the accuracy of both our nuclear data processing codes and our Monte Carlo transport codes, while avoiding differences due to the use of different sets of nuclear data, since both of our codes used the same TART 2005 data.

Comparison Results

In the earlier study [3] we were only able to compare one simple integral parameter, K-eff. The comparisons that we performed for this report are much more stringent, in that we compared both,
1) Integral parameters, K-eff, neutron lifetime, and decay constant, and,
2) Differential neutron production and absorption spectra.

Also in order to illustrate the differences we present results using continuous energy cross sections, and unshielded 616 group Multigroup cross sections, as well as free and bound atom thermal scattering law data.

Integral Results

The following tables present MERCURY and TART results for twelve (12) problems: three different uranium pin radii, free and bound thermal scattering, continuous energy and multigroup cross sections. Results for three integral parameters are presented: K-eff, the neutron removal lifetime, and the system time constant (α).

In general K-eff is defined as the ratio of neutron production to neutron removal,

$$\text{K-eff} = \frac{\text{Production}}{\text{Removal}} = \frac{\text{Production}}{[\text{Absorption} + \text{Leakage}]} = \frac{\text{Production}}{\text{Absorption}}$$

These pin-cell problems involve an infinite repeating lattice of cells, so there is no leakage from the system, and as such K-eff is simply the ratio of neutron production to absorption.

The results for both codes are based on using 10^8 (100 million) source neutrons. K-eff and neutron removal lifetime are based on the accumulated statistics for all of the neutrons. The results below indicate that the difference between the results for the two codes is roughly the same as the statistical uncertainty assigned by each code to its results. In other words, the results for both codes are statistically identical. Compared to the large spread in K-eff values of over 2% we found in ref. [3], here the differences are closer to the 0.01% level, two orders of magnitude smaller than in ref. [3]. The results for the neutron removal lifetime are also in excellent agreement, also close to the 0.01% level of difference.

Unlike K-eff and neutron removal lifetime which are calculated directly from accumulated statistics, the system time constant is a derived quantity defined as,

Time constant α = [K-eff – 1]/[Removal lifetime]

Since this involves the difference [K-eff – 1], we expect this quantity to be less accurate, particularly for any system where K-eff is close to unity, as it is in all of these pin-cell problems. Given this limitation, the results are in excellent agreement, in eleven (11) cases differing by less than 1%, and in only one case exceeding this, because K-eff is so close to unity that the result is a great deal of round-off.

K-eff

Type	1/2" Free	1/2" Bound	1/4" Free	1/4" Bound	1/8" Free	1/8" Bound
Continuous						
TART	1.01084	0.96015	1.01044	0.91470	1.01174	0.90286
MERCURY	1.01091	0.96035	1.01049	0.91475	1.01178	0.90293
Difference	0.00007	0.00020	0.00005	0.00005	0.00004	0.00007
%	0.007	0.020	0.005	0.005	0.004	0.007
Multigroup						
TART	0.97455	0.92581	0.99873	0.90418	1.01072	0.90222
MERCURY	0.97444	0.92575	0.99888	0.90432	1.01065	0.90251
Difference	0.00011	0.00006	0.00015	0.00014	0.00007	0.00029
%	0.011	0.006	0.015	0.014	0.007	0.029

Removal Lifetime (microseconds)

Type	1/2" Free	1/2" Bound	1/4" Free	1/4" Bound	1/8" Free	1/8" Bound
Continuous						
TART	56.9773	63.4182	90.8117	101.035	102.771	113.462
MERCURY	56.9709	63.4059	90.8142	101.045	102.746	113.455
Difference	00.0064	00.0123	00.0025	000.010	000.025	000.007
%	0.011	0.019	0.003	0.010	0.024	0.006
Multigroup						
TART	54.7235	60.9282	89.7432	99.8575	102.195	112.851
MERCURY	54.7125	60.9086	89.7001	99.8191	102.186	112.782
Difference	00.0110	00.0196	00.0431	00.0384	000.009	000.069
%	0.020	0.032	0.043	0.038	0.009	0.061

Time Constant (α) (milliseconds) = [K-eff – 1]/[Removal Time]

Type	1/2" Free	1/2" Bound	1/4" Free	1/4" Bound	1/8" Free	1/8" Bound
Continuous						
TART	0.19025	-0.62829	0.11499	-0.84419	0.11421	-0.85613
MERCURY	0.19145	-0.62539	0.11555	-0.84367	0.11468	-0.85555
Difference	0.00120	0.00290	0.00056	0.00052	0.00047	0.00058
%	0.630	0.461	0.487	0.062	0.411	0.068
Multigroup						
TART	-0.46500	-1.2177	-0.01420	-0.95973	0.10488	-0.86637
MERCURY	-0.46712	-1.2189	-0.01250	-0.95853	0.10422	-0.86434
Difference	0.00212	0.0012	0.00170	0.00120	0.00066	0.00197
%	0.456	0.098	11.97	0.125	0.629	0.277

Effects of Models

There are physically only three different pin-cells, and with each we used a combination of models, including: continuous or multigroup cross sections and bound or free atom thermal scattering. Here we compare TART results for each of the three pin-cells, grouping together results for all of the models used.

As an illustration of how important it is to include thermal scattering, in the below table we include results for the cases when thermal scattering is not included; in the below table this is identified as "none". This case corresponds to treating the target nuclei as stationary, so that neutrons will continue to slow down to the lowest limit of our nuclear data (10^{-11} MeV).

Model	1/2"	1/4"	1/8"
Continuous Bound	0.96015	0.91470	0.90286
Continuous Free	1.01084	1.01044	1.01174
Continuous None	0.83169	0.79988	1.01685
Multigroup Bound	0.92581	0.90418	0.90222
Multigroup Free	0.97455	0.99873	1.01072
Multigroup None	0.76426	0.77223	1.00732
Maximum	1.01084	1.01044	1.01174
Minimum	0.76426	0.77223	0.90222

We can see that the answers strongly depend on the combination of modes used; here we consider Continuous Bound to be the "best" model. For these pin cells we can summarize the effects of the model used as follows,

1) **Thermal scattering** – Without thermal scattering (none) there is an enormous difference between the" best" of these values, and the effect is unpredictable, i.e., for the 1/2" and 1/4" radius pin "none" grossly under predicts the value of K-eff, whereas for the 1/8" case it over predicts K-eff. The important point to note is that when we look at the actual energy dependent production and absorption (see the figures below), without thermal scattering the spectra are completely unrealistic, so that whatever answers this method produces will be totally unreliable.

2) Continuous versus Multigroup – This has a significant effect on K-eff, particularly for the 1/2" pin case, which contains the highest concentration of U238. In comparison for the 1/8" pin case it has much less effect. Here the 1/2" pin case is more typical of low enriched uranium (LEU) fuel, and these results show the heterogeneous effect of self-shielding, even here where we used 616 groups.

3) Bound versus Free – For these pin cells the difference in K-eff between bound and free ranges from roughly 5% for the 1/2" case to 10% for the 1/8" case. It should be noted that these pin cells were designed to test the effect of thermal scattering models, and as such the effect here is more than in a typical water moderated reactor where it is closer to 1%; small but not at all insignificant.

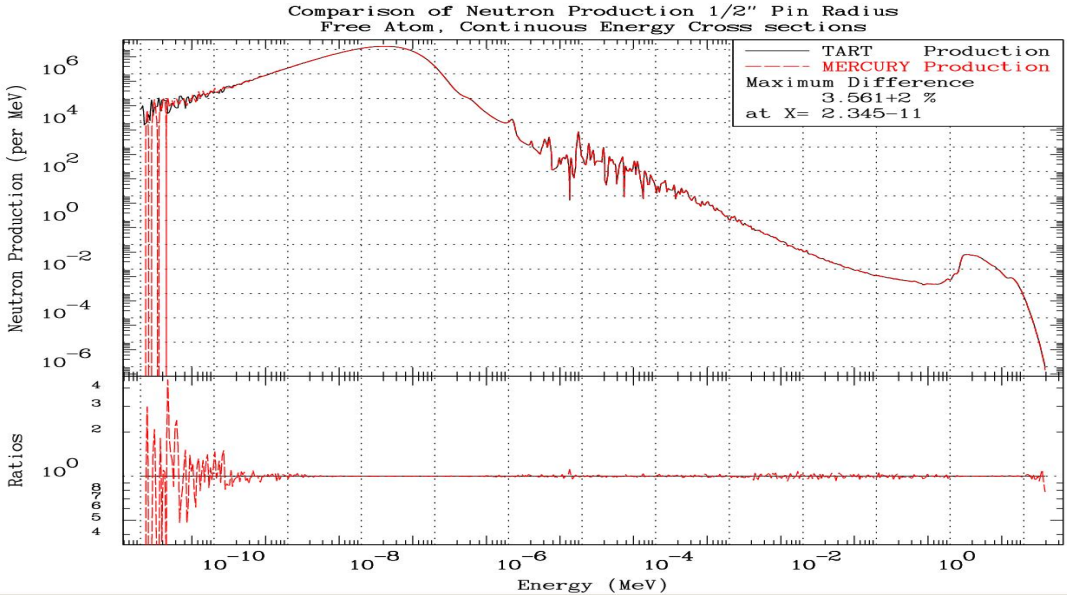
Differential Results

As described above for these pin-cells there is no leakage, and as such K-eff is simply the ratio of neutron production to absorption,

$$\text{K-eff} = \frac{\text{Pr}\,oduction}{Absorption}$$

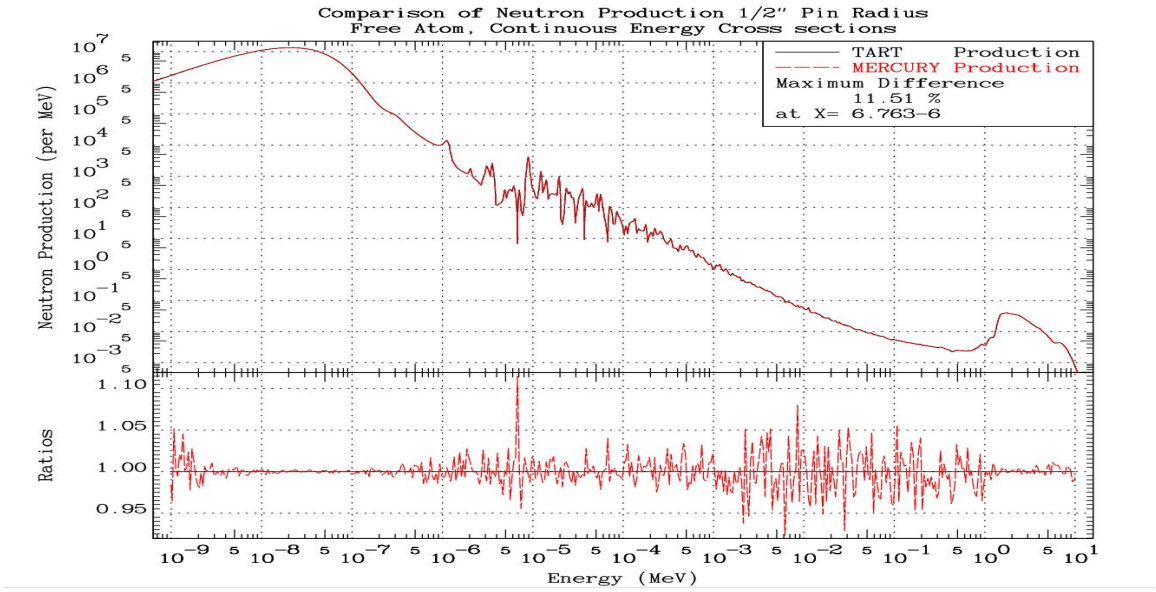
In additional to the simple scalar K-eff, we also calculated energy dependent production and absorption spectra, using the TART tally bin structure, of 50 groups per energy decade equally spaced in the log of energy between 10^{-11} MeV and 20 MeV, resulting in 616 energy tally bins. It is encouraging that we found such excellent agreement for K-eff, but experience has demonstrated that this is a necessary, but not a sufficient, condition to insure our codes are really correctly modeling our systems. For example, see the example near the end of this report showing results for two codes that had excellent agreement in K-eff, and yet very poor agreement in the energy dependent neutron production and absorption.

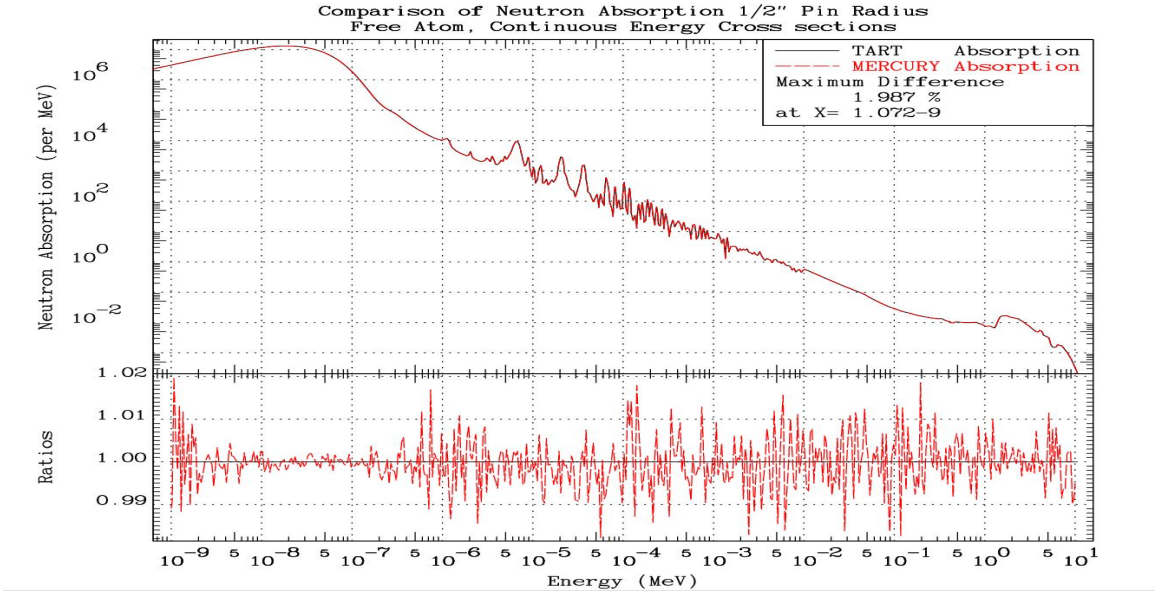
The first plot below is of the neutron production over the entire energy range. For these problems we expect to find very few neutrons below roughly 10^{-9} MeV or above 10 MeV, which is shown by the large statistical error in the results. These energy ranges do not make any significant contribution to the production and absorption, and will be ignored in all following figures, in order to allow us to see differences in more detail.



1/2" Pin Radius, Free Atom Data, Continuous Energy Cross Sections

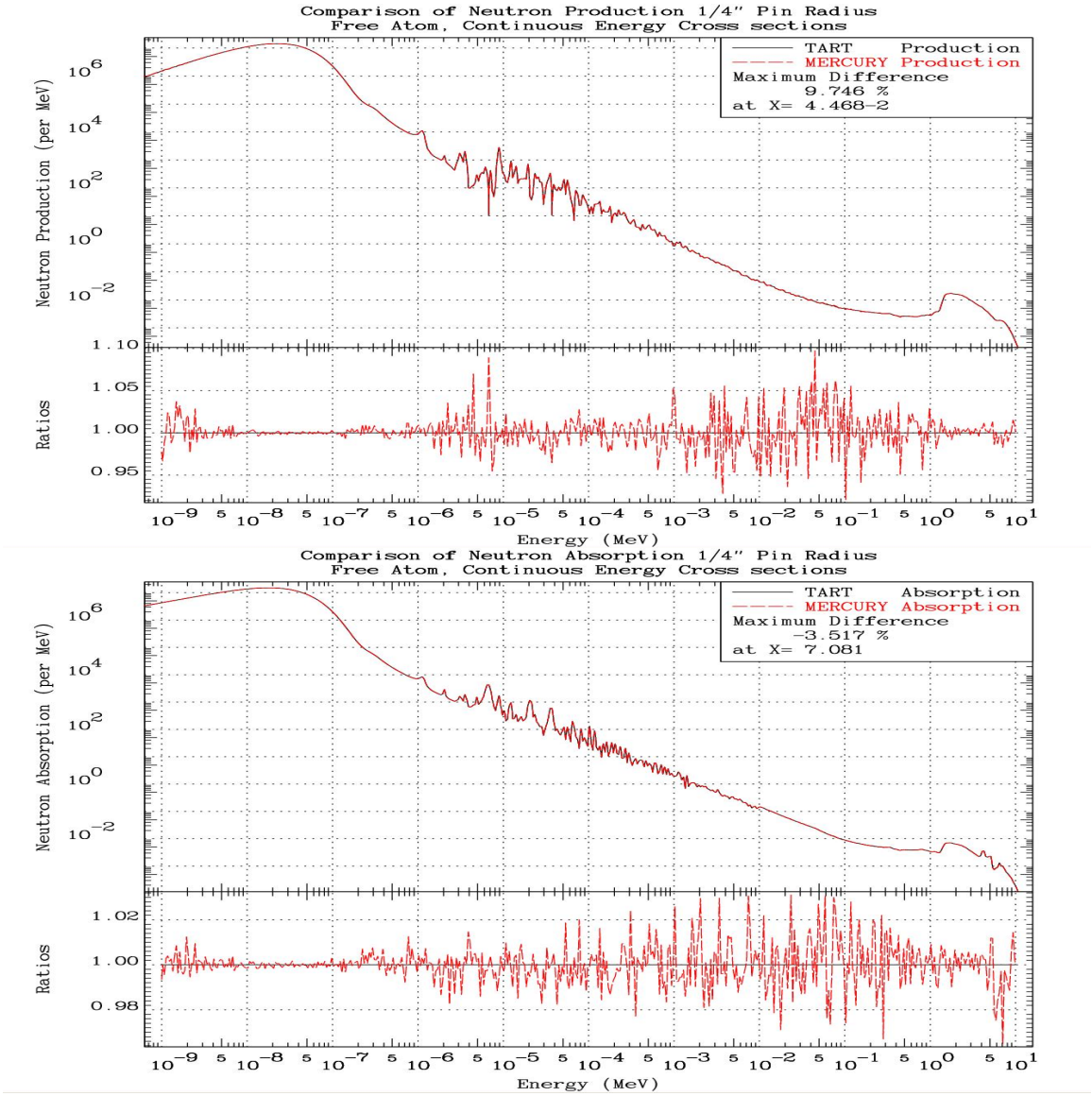
Once we restrict the energy range, we can see that we have excellent agreement over the entire energy range for both production and absorption. In most cases the differences are 1% or less, with a few exceptions near resonances, where self-shielding depresses production near some strong U238 capture resonance. For example, note the 11% difference in production over a very narrow energy range near 6 or 7 eV. Here the production is orders of magnitude lower than at nearby energies, making it statistically difficult to accurately sample. Fortunately, minima such as this contribute little to the overall production integral, and as such have essentially no effect on K-eff.





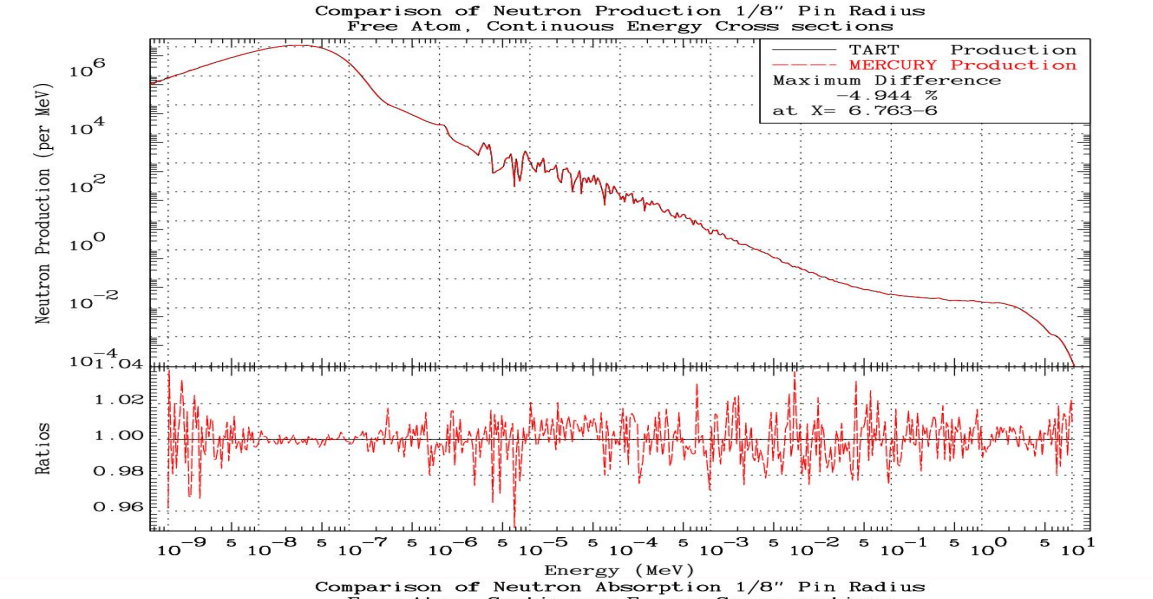
1/4” Pin Radius, Free Atom Data, Continuous Energy Cross Sections

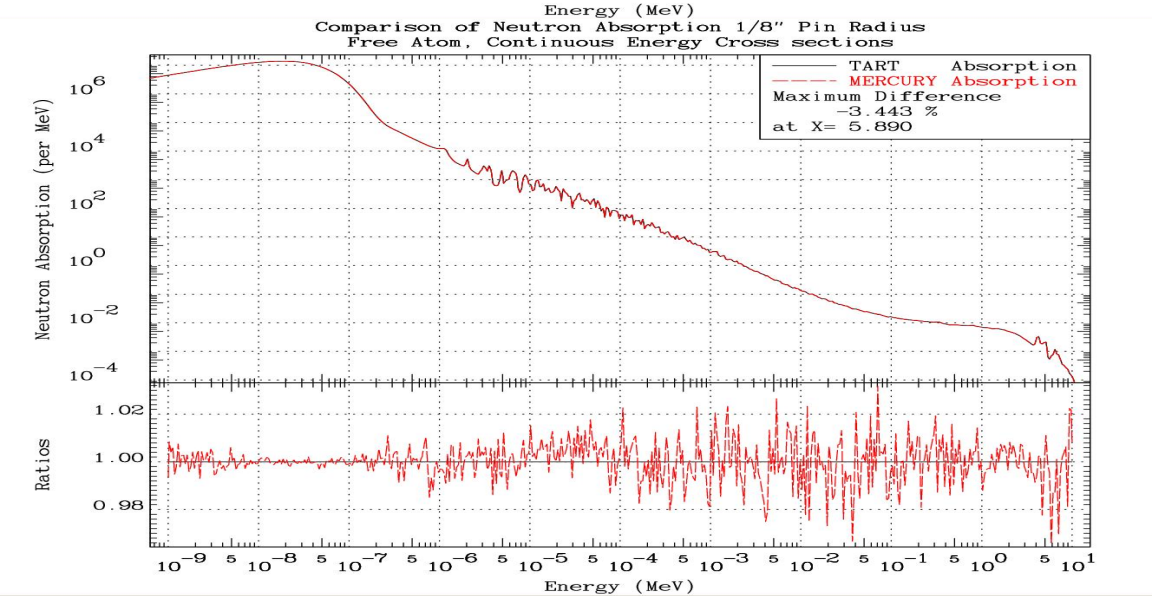
When we compare the 1/2" and 1/4" radius pin results they are not surprisingly very similar. Compared to the 1/2” case, the 1/4" pins contain less U238 so that the production is not depressed as much in the 6 to 7 eV energy range. Overall the agreement is again excellent.



1/8” Pin Radius, Free Atom Data, Continuous Energy Cross Sections

When we compare the 1/8" radius pin results to the other two cases we find very similar results. The 1/8" pins contain much less U238 so that the production is not appreciable depressed in the 6 to 7 eV energy range. Overall the agreement is again excellent.



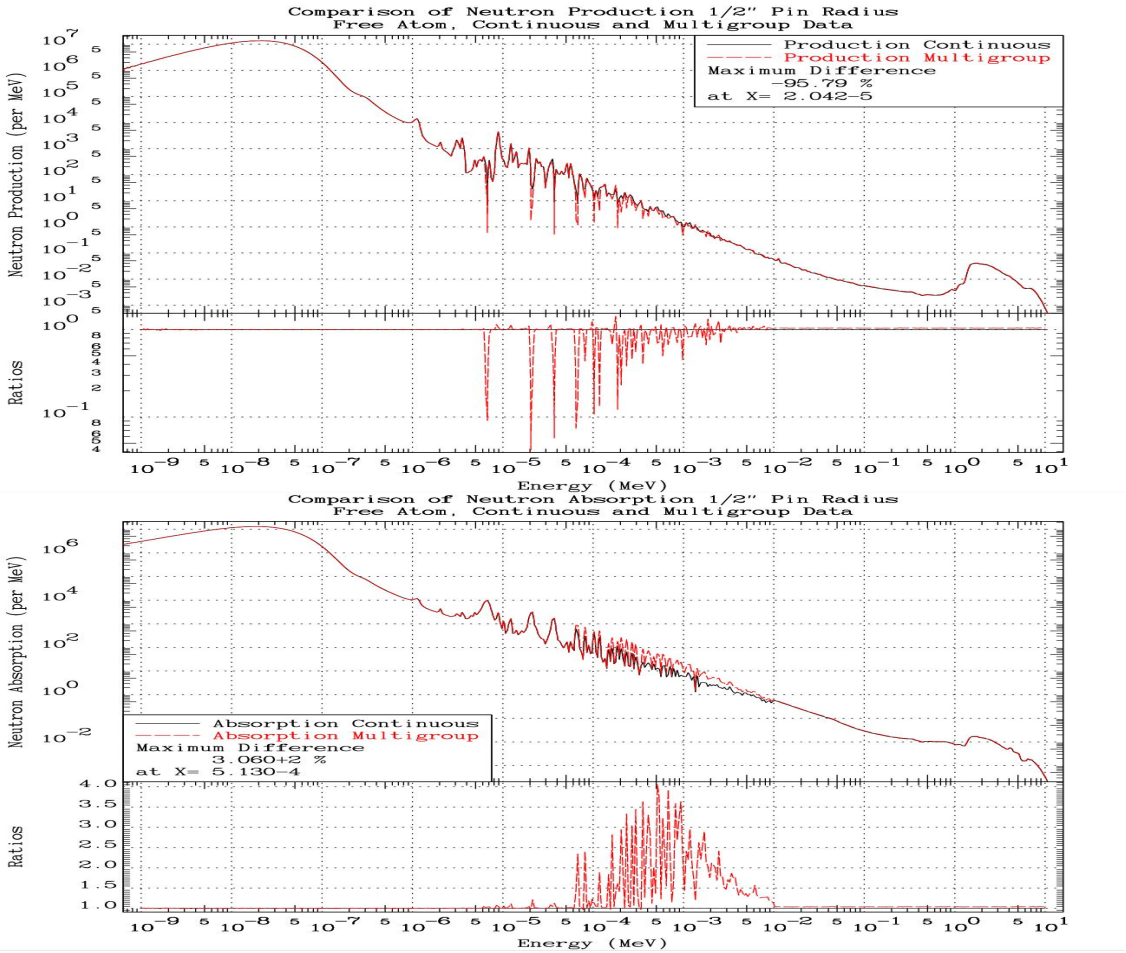


There is little to be gained by including plots of the other cases; all cases show similar excellent agreement between the MERCURY and TART energy dependent production and absorption spectra. However, it is interesting to compare results using the same code and different models. Therefore here we compare TART results for the 1/2" radius pins, free atom data, using continuous energy and Multigroup results using 616 energy groups. Then we compare results using free versus bound atom data.

Self-Shielding: Continuous Energy vs. Multigroup Results

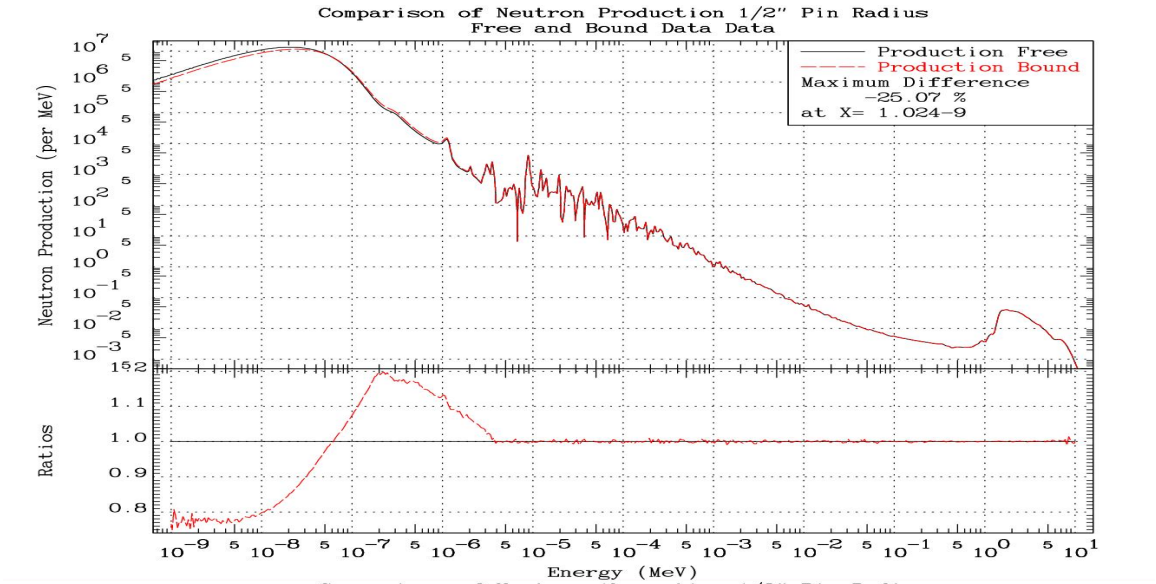
The below figures illustrates that what might seem like a large number of groups, 616, are in this case no where near enough to account for the resonance self-shielding. In this case the unshielded multigroup cross sections are too big, particularly the U238 capture cross sections. U238 only significantly fissions in the MeV energy range; below this range it is a strong neutron absorber. So that what we see in both production and absorption spectra is the effect of U238 capture resonances in the eV and keV energy range: these depress production and increase absorption, which is exactly the effect that we see.

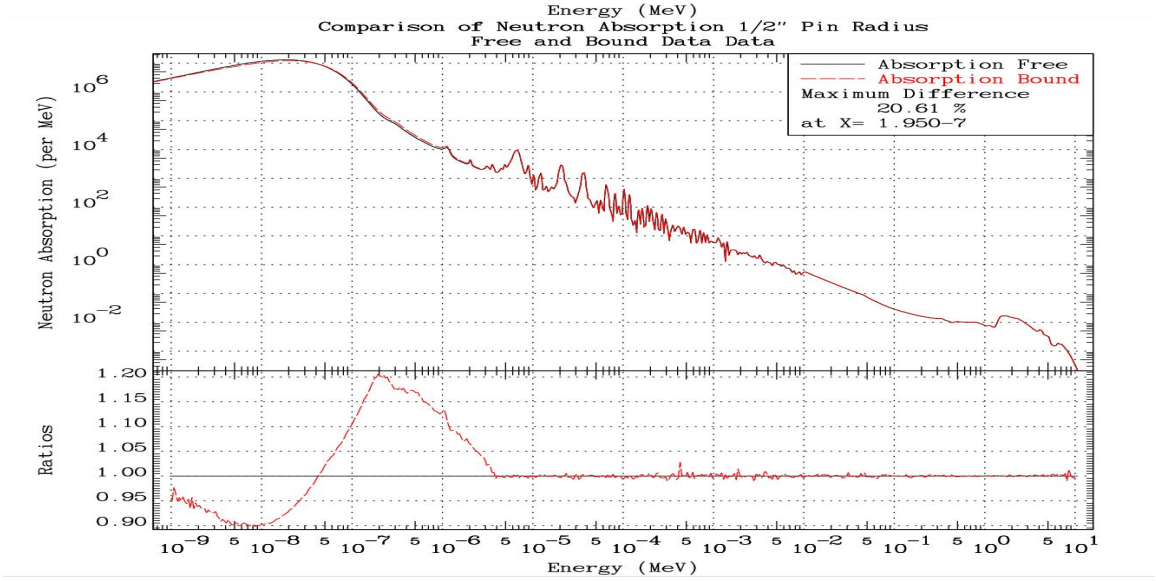
Using continuous energy cross section we calculate K-eff = 1.01084, whereas when we use Multigroup cross sections we calculate K-eff = 0.97455; the difference is a reduction in K-eff of roughly 3.6%, which is enormous compared to the other differences we have found. Most important to realize is that these results show how dangerous using a poor model can be: here using accurate continuous energy cross sections predict this system is dangerously super-critical, whereas using less accurate multigroup cross sections predict this system is safely sub-critical. **What we learn from these results is that whenever possible use continuous energy cross sections; when forced to use the multigroup method you must account for self-shielding even when using many groups.**



Free vs. Bound Atom Thermal Scattering Results

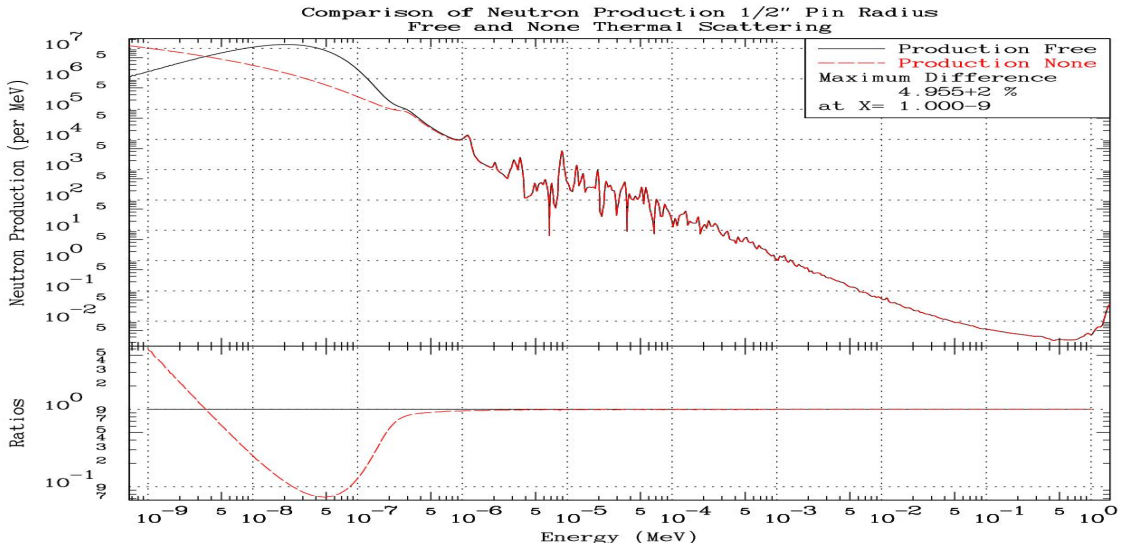
Another case to compare is free versus bound atom thermal scattering data. The figures below illustrate that the hydrogen bound data only extends up to about 4 eV; above this point free and bound results are identical. Below 4 eV there are large differences in both production and absorption. Binding tends to shift the spectra to a slightly higher energy. Using free atom data, K-eff = 1.01084, whereas with bound atom data, K-eff = 0.96015, for a decrease in K-eff of over 5%. For the 1/4" and 1/8" cases the change is even larger, with over a 10% difference for the 1/8" case. **What we learn from these results is the importance of using bound atom data.**

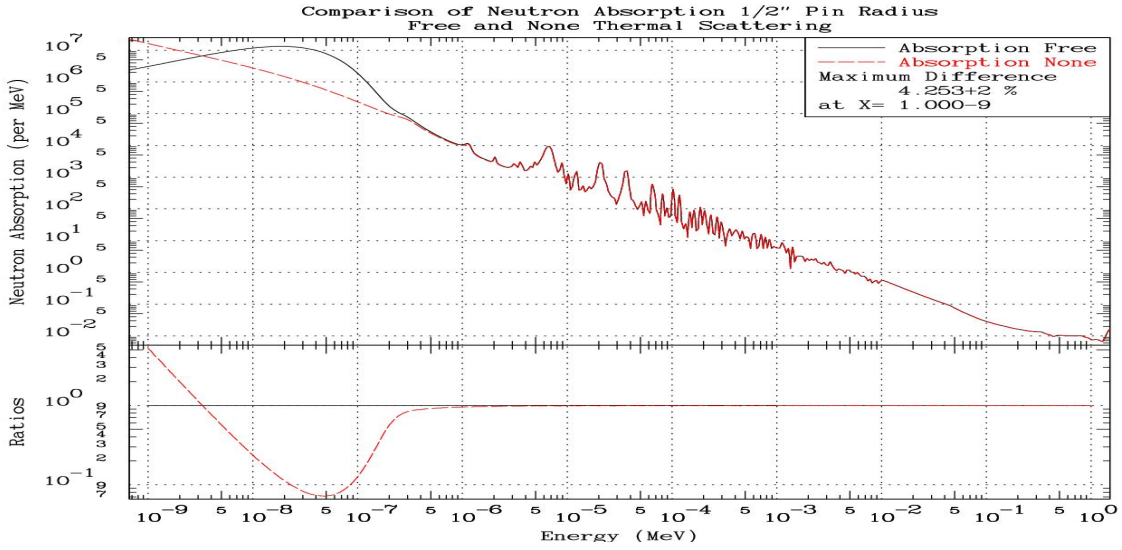




Free Atom vs. No (None) Thermal Scattering Results

The last case to compare is free atom versus no (none) thermal scattering data. If we look in detail the figures below illustrate that the effect of free atom scatter extends up to about 100 eV; above this point free and no results are identical. Below 100 eV there is only a small difference between the two results down to about 1 eV. Below 1 eV the results rapidly diverge, with the free atom results going over into a Maxwellian-like thermal spectrum. In contrast with no thermal scattering the neutrons continue to slow down in an unrealistic shape all the way to the lower limit of our nuclear data (10^{-11} MeV); this maximizes absorption in the water, greatly decreasing K-eff. **What we learn from these results is the importance of using thermal scattering data; at least free atom and where available bound atom.**





Conclusions

We have verified that MERCURY can accurately model both free atom and bound atom neutron thermal scattering. This was accomplished by comparing MERCURY [1] and TART [2] results, for a series of reactor pin-cells, that were earlier calculated by a number of Monte Carlo transport codes [3]. For decades TART has been compared to other codes and found to be in excellent agreement. In particular, in this earlier study [3] TART performed very well compared to these other codes, and TART is here used as a standard to which MERCURY results are compared.

Compared to the spread in the results found in the earlier study [3], here the agreement between MERCURY and TART results are incredible. Even for simple scalar integral parameters, such as K-eff, in this earlier study differences of up to over 2% were found. Here the differences in K-eff between MERCURY and TART results are closer to 0.01%, two decades smaller than the differences seen in the earlier study [3].

Here we present the results of our MERCURY vs. TART comparisons and we also explain how we were able to obtain such incredible agreement. Lastly we illustrated the importance of using thermal scattering law data.

From our earlier study [3] we found that the differences in results were traced to four major factors,

1) Differences between the sets of nuclear data used.
2) The accuracy of nuclear data processing codes.
3) The accuracy of the models used in our Monte Carlo transport codes.
4) Code user selected input options.

Here we avoided most of these problems by,

1) Both codes used exactly the same nuclear data, namely the TART 2005 data.
2) Each code used its own nuclear data processing code. Even though these two data processing codes are independent, they have been extensively tested to insure the processed output results closely agree.
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4) Both codes used the same input options; both modeled the geometry and materials in exactly the same manner; both used the same number of neutron histories to produce results to within comparable statistical accuracy.

These constraints were used to test the accuracy of both our nuclear data processing codes and our Monte Carlo transport codes, while avoiding differences due to the use of different sets of nuclear data, since both of our codes used the same TART 2005 data.

References

[1] **MERCURY:** MERCURY User Guide (Version b.8), Lawrence Livermore National Laboratory, Report UCRL-TM-204296, Revision 1, by R. J. Procassini and J. M. Taylor, (2005), more information concerning MERCURY is available online at http://www.llnl.gov/mercury

[2] TART05: A Coupled Neutron-Photon 3-D, Combinatorial Geometry Time Dependent Monte Carlo Transport Code, UCRL-SM-218009, Lawrence Livermore National Laboratory, by Dermott E. Cullen, November 2005, available online at http://www.llnl.gov/cullen1/mc.htm

[3] "How Accurately can we Calculate Thermal Systems", UCRL-TR-203892, Lawrence Livermore National Laboratory, by Dermott E. Cullen, et al., April 2004.; now available on-line at http://www.llnl.gov/cullen1/pin_cell.htm

Appendix A

Pin-cell Models

The following is the description of the theoretical pin-cell problems from ref. [3], here somewhat edited to meet our current needs. Differences from the original are shown here in a red font.

Ground rules

I want to test each code package completely, including the important, and yet often overlooked influence of code users on code results. In order to do this I ask each participant to assume they are the local expert on a code. Someone comes to your office and asks you what your best estimate is of K-eff for a system, using thermal scattering law data or free atom scattering. They are not experts on neutron transport or your code, so they only define the geometry and materials. You, as the local code expert, must then make all decisions as far as what nuclear data to use and what input parameters to define for your code, and supply the requested K-eff. If you routinely use more than one nuclear data library, or would like to show results using a variety of input options, feel free to send more than one set of results using each of your data libraries or input options; in this case please clearly state what data and input options were used for each set of results, so that we can distinguish between your sets of results. **For this report this ground rule was changed to insure that MERCURY and TART both used the same nuclear data.**

My Simplest Possible Infinite Repeating Lattice of Uranium/Water Cells

To simulate a water-moderated, uranium fueled, thermal reactor, we can use a simple cylindrical uranium pin, centered in and surrounded by a square cell filled with water. To simulate an infinite array of cells we make the four sides of the square totally reflecting, i.e., no leakage. The third dimension of the cell, along the axis of the cylinder, can be either infinite in extent, or finite with reflecting surfaces, whatever is easiest for your code to handle. The net effect is a system that is infinite in all directions, so there is no leakage, and infinitely repeats the cylindrical pin surrounded by water. As far as K-eff is concerned, in this system we need only be concerned with neutron production and absorption; again, there is no leakage.

Below I illustrate a 1/4" (0.635 cm) radius uranium cylinder (the red zone), surrounded by a 2" (5.08 cm) square filled with water (the green zone). For our use here it is sufficient to maintain the 2" pitch, as well as the density of fuel and water, and ONLY vary the radius of the pin, and U^{235} to U^{238} ratio to make the system near critical, i.e., K-eff ~ 1.0, using Free Atom thermal scattering. In each case we will then change only one input parameter to use either Free Atom or $S(\alpha,\beta)$ thermal scattering law data. In this manner we can be sure that any differences in K-eff and neutron spectrum are due ONLY to the difference in the thermal scattering model used.

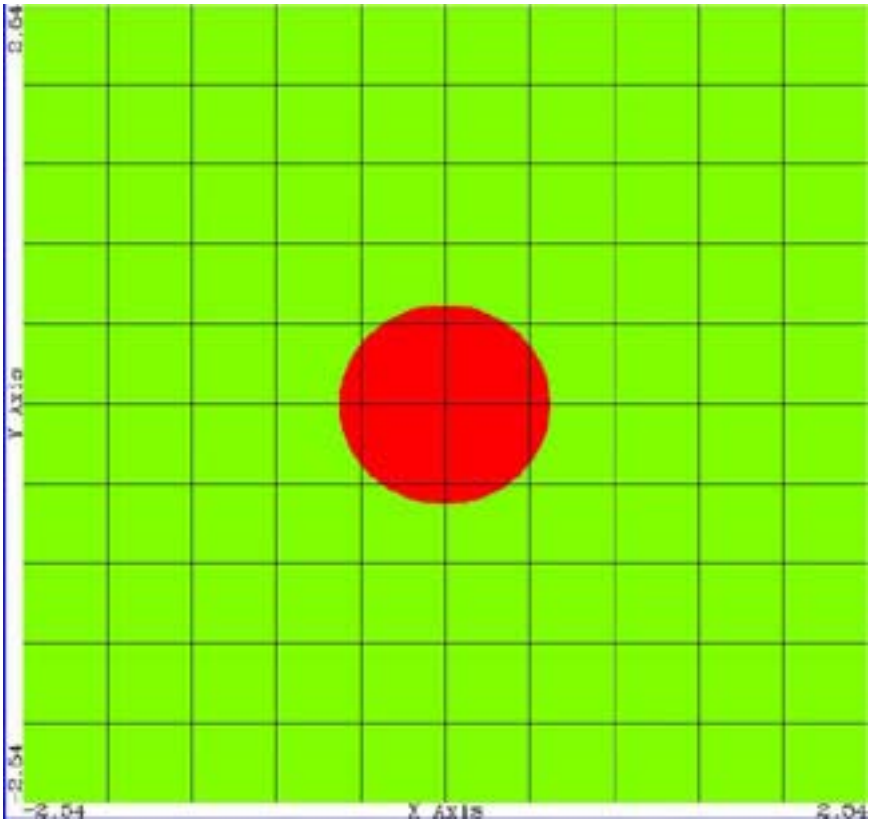


Fig. 1: 1/4” radius fuel pin, in 2” square water cell

I propose three different pin cell problems, and for each you are asked to estimate K-eff using thermal scattering law data or free atom data; therefore there are a total of six problems. In all cases the problem is a square 2” (5.08 cm) cell filled with water at 1.0 grams/cc density, containing a cylindrical fuel pin at 18.8 grams/cc density, and a radius of 1/2”, 1/4” or 1/8”, where the U^{235} and U^{238} ratio has been varied to make the system near critical using free atom data. Results should be calculated using both free atom and S(α, β) thermal scattering law models.

Please remember that these are only theoretical problems that simulate the effects we are interested in. For simplicity in analyzing results the fuel is composed only of U^{235} and U^{238}, and there is no cladding or air gap. The ratio of water to fuel has been defined to maximize the effect of thermal scattering, since this is the effect we are interested in.

I ask that contributors submit answers for these problem, and only these problems, so that they can be meaningfully compared to answers from other codes. Please, do not try to be creative and make changes to these specifications; unless your answers correspond to exactly these problems we cannot use your answers.

Contributors can send any number of sets of results; we are particularly interested in results using different nuclear data libraries or input options with the same transport code **– again, not for this report where we use only one set of nuclear data.**

It is worth noting that the test cases used here are not exactly representative of commercial power reactors where the pitch is typically about 1.25 cm = ~0.5" and pin radius less than .5 cm = ~0.2". Such systems are somewhat less sensitive to the thermal scattering law data. Since the primary topic of this paper is the effect of thermal scattering, we have defined theoretical systems in which the effects of thermal scattering are maximized; the test cases here are similar, but not identical to actual commercial power reactors.

All three problem include water surrounding the central fuel pin

2" square water - 1.0 grams/cc density
2.0 atoms of hydrogen to 1.0 atoms of oxygen

Below I describe each of the three problems, highlighting how they differ from one another.

Problem #1

1/2" (1.27 cm) radius fuel pin – 18.8 grams/cc density – total $<\nu>$ - static criticality
99.02 atoms of U^{238} to **0.98** atoms of U^{235}

Problem #2

1/4" (0.635 cm) radius fuel pin – 18.8 grams/cc density – total $<\nu>$ - static criticality
96.5 atoms of U^{238} to **3.5** atoms of U^{235}

Problem #3

1/8" (0.3175 cm) radius fuel pin – 18.8 grams/cc density – total $<\nu>$ - static criticality
30.0 atoms of U^{238} to **70.0** atoms of U^{235}

Basic Definitions

When I was in graduate school one of my professors said that there are more definitions of reactor parameters than fleas on a dog. I had completely forgotten about this statement until I started this study. Even for something as seemingly simple as K-eff the various codes uses different definitions, differing mostly in how they handle non-fission, multiple neutron emission, such as (n,2n), (n,3n), etc. These different definitions of K-eff lead quite naturally to different definitions of quantities such as the median fission energy, neutron lifetime, or removal time, as well as different production, absorption and leakage energy dependent spectra. I'll try to explain the differences in the appendix. For now it is sufficient for the reader to know that differences in the basic definitions of K-eff will lead to slightly different values of K-eff even if we are using deterministic codes where there are no statistical uncertainties. At least for this study these differences are small compared to the differences that we see in values of K-eff calculated by each code, so that for our comparison of integral parameters we need not be concerned in this paper.

This is not a problem when comparing MERCURY and TART, because both use exactly the same consistent definition of K-eff and the other parameters studied here; see, the appendix for a description of alternative definitions of K-eff, etc.

Using Thermal Scattering Law Data

You might think that it would be sufficient if a code designer uniquely defines the basic data they used, as for example by saying: I used the ENDF/B-VI thermal scattering law data, but it isn't. One interesting result of this comparison was to discover how many different interpretations there are of the same basic data in each code. Some codes sample $S(\alpha,\beta)$ data directly, some convert it to continuous double differential data in secondary energy and scattering cosine, some convert it to discrete data in secondary energy and direction, and some use a multi-group representation. Our results indicate that all of these representations can accurately reproduce a simple integral parameter, such as K-eff. It remain to be seen whether or not the detailed differences in the energy dependent neutron flux effect other parameters of interest; this is outside the scope of the current study, but suggests possible follow-on studies; **see the end of appendix B.**

Bound versus Free Atom

In this report we present results using two different models of thermal scattering. The first model uses thermal scattering law data, $S(\alpha,\beta)$. With this model thermal scattering can include atomic translational motion as well as vibration and rotation. The second model uses free atoms, in which we assume the thermal atomic motion is Maxwellian. Both bound and free models include *a priori* and *a posteriori* affects. The *a priori* affect is that the thermal motion changes the relative speed between target atoms and incident neutrons, which means that the reaction rate is changed; this effect is accounted for by Doppler broadening the cross sections, e.g., see the below plot of the hydrogen cross section that show the affect of Doppler broadening. The *a posteriori* affect is that the thermal motion changes the secondary direction and speed of scattered neutrons; this is where the bound and free models really differ. In order to correctly calculate our example problems *a priori* and *a posteriori* affects must both be included in the neutron transport calculation. For purposes of this report we define the terms free atom and free gas to be synonymous; we assume that both refer to a model in which atoms have a thermal motion that can be described by a Maxwellian; this motion is used both *a priori* to Doppler broaden cross sections and *a posteriori* to describe the distribution of secondary neutrons in direction and energy.

Appendix B

This appendix is basically a copy of the appendix from ref. [3], here slightly modified to meet our current needs. Here we define K-eff that both MERCURY and TART use, and also define the 616 energy group tally structure that we used for all detailed comparisons in this report. These definitions will be useful to anyone who wishes to use different Monte Carlo code(s) to model these pin-cells, and compare to the MERCURY and TART results.

Definition of K-eff

For time independent codes there is a very simple textbook definition that can be used to define K-eff. It is the ratio of the number of neutrons produced by fission in one generation to the number produced in the preceding generation; these codes need not consider anything else. For time dependent codes or codes that define K-eff in terms of a balance between neutrons produced and removed this is more complicated, because fission is not the only process that can produce neutrons during a generation; there is also (n,2n), (n,3n), etc., and how codes handle these lead to different definition of K-eff. Below I'll explain the differences.

Starting from the time dependent, linear Boltzmann equation in general geometry,

$$\frac{1}{v}\frac{\partial N}{\partial t} + \Omega * \nabla N + \Sigma t * N = \iint (< \nu > \Sigma f + \Sigma scatter + 2\Sigma n,2n + 3\Sigma n,3n + ...) N d\Omega' dE'$$

Where $N(r,\Omega,E,t)$ is the neutron flux, $v * n(r,\Omega,E,t)$, v is the neutron speed, Σt is the macroscopic total cross section, $< \nu >$ is the average number of neutrons emitted per fission, Σf, $\Sigma scatter$, $\Sigma n,2n$, $\Sigma n,3n$, etc., are the macroscopic cross sections for each type of event. For simplicity I will use neutron density $n(r,\Omega,E,t)$ in the following,

Integrate over all space, energy, and direction

$$\frac{\partial n}{\partial t} + [\, L * v * n \,] + [\, \Sigma t * v * n \,] = [(< \nu > \Sigma f + \Sigma scatter + 2\Sigma n,2n + 3\Sigma n,3n + ...) v * n]$$

Collecting terms together we find a simple equation defining the time dependent behavior of the system,

$$\frac{\partial n}{\partial t} = \alpha * n$$

$$\alpha = [(< \nu > \Sigma f + \Sigma scatter + 2\Sigma n,2n + 3\Sigma n,3n + ...) v] \; - \; [L * v] \; - \; [\Sigma t * v]$$

= [Production rate] – [Removal Rate]

The time constant (α) is a physical observable and as such has a unique value that we can determine. The non-uniqueless of K-eff and related terms is because exactly the same terms appear in this definition of α as positive and negative terms that we can completely cancel (scatter), or as simply related terms that we can partially cancel (n,2n).

I will divide the total cross section by events according to how many neutrons result from each type of event: **none** – capture, (n,p), (n,a), etc., **one** – scatter, (n,np), (n,na), etc., **more than one** – fission, (n,2n), (n,3n), etc.. All of those events that result in one neutron do not directly effect the neutron balance of the system (they effect it indirectly through the leakage), and appear in exactly the same form in this definition as positive and negative terms, so that we can cancel them. Upon cancelling scatter, (n,np), (n,na), etc.,

$$\alpha = [(<\nu>\Sigma f + 2\Sigma n,2n + 3\Sigma n,3n + ...)v] - [L * v] - [(\Sigma n,0 + \Sigma f + \Sigma n,2n + \Sigma n,3n + ...) * v]$$

Up to this point all or least most of the codes use the same definitions, and this is the definition that TART uses, i.e., any event that introduces additional neutrons into the system is considered production, and any event that produces neutrons also removes neutrons, etc., (n,2n) removes one neutron and produces two neutrons,

Production rate = $[(<\nu>\Sigma f + 2\Sigma n,2n + 3\Sigma n,3n + ...)v]$
Removal Rate = Leakage + Absorption = $[L * v] + [(\Sigma n,0 + \Sigma f + \Sigma n,2n + \Sigma n,3n + ...) * v]$

Other codes change this to agree with the textbook definition of K-eff where production is only due to fission. This requires them to subtract $2\Sigma n,2n + 3\Sigma n,3n + ..$ from the production and removal resulting in the definitions,

Production rate = $[(<\nu>\Sigma f)v]$
Removal Rate = $[L * v] + [(\Sigma n,0 + \Sigma f - \Sigma n,2n - 2\Sigma n,3n - 3\Sigma n,4n - ...) * v]$

Note, that we still have exactly the same definition of the physically observable time constant (α), and for an exactly critical system K-eff remains unity using any of these definitions. Regardless of how they define production and removal, the codes define,

$$\alpha = [\text{Production Rate}] - [\text{Removal Rate}] = [\frac{\text{Production}}{\text{Removal}} - 1] * [\text{Removal Rate}]$$

$$= [\text{K-eff} - 1]/Tr \qquad Tr = \text{Removal Time}$$

$$\text{K-eff} = \frac{\text{Production}}{\text{Removal}} \qquad \text{Removal Time} = 1/[\text{Removal Rate}]$$

Here we can see that even though the time constant (α) has a unque definition, K-eff and the removal time, do not, since all codes do not define production and removal the same way. With the TART definition any event that produces more than one neutron ends a

generation, and adds to the removal $\Sigma f + \Sigma n,2n + \Sigma n,3n + ...$ and adds to the production $< \nu > \Sigma f + 2\Sigma n,2n + 3\Sigma n,3n + ...$ Codes that do not consider that $(n,2n),(n,3n)$, etc., end a generation, add nothing to production for these events and subtract from the removal $\Sigma n,2n + 2\Sigma n,3n + 3\Sigma n,4n + ...$

As a quantitative example by Andrej Trkov for WIMS, the K-eff from codes, which adopt the convention of defining production from fission alone require a correction, which is easily implemented for the "no leakage" case. We must add $2\Sigma n,2n + 3\Sigma n,3n + ..$ to the production and removal and using the absorption as a normalization results in the definitions,

K-eff = (K-eff* + 2$\Sigma n,2n/\Sigma a$ + 3$\Sigma n,3n/\Sigma a$ + …)/(1 + 2$\Sigma n,2n/\Sigma a$ + 3$\Sigma n,3n/\Sigma a$ + …) ,

Here Σa is the absorption cross section (including fission). The ratios $\Sigma n,2n/\Sigma a$ calculated with WIMS-D for the three cases are:

½"	0.00182
¼"	0.00083
1/8"	0.00032

From the above it follows that the correction amounts to 0.00015 for the ½" bound case and smaller for all other cases; in other words, it is well below the integral differences we see in this study, and yet important when we try to compare energy dependent spectra. It is worth noting that even in the case of the very thermalized systems, because fission at any energy creates fission neutrons above the (n,2n) threshold, (n,2n) accounts for a few tenths of a per-cent of the total neutrons produced in these systems; it is even higher for faster neutron systems. Therefore in terms of the overall neutron economy it is not an effect that can be simply ignored.

Where do we go from here: Proposed Future Detailed Comparisons

I propose that in the future we perform more detailed comparisons, including the production, absorption, and leakage energy dependent spectra. In order to do this we all need to use the same definitions.

Any of the above definitions is physically acceptable, and in most situations the calculated integral parameters, such as K-eff are very similar, but differences do create a problem if we are to compare production, absorption and leakage energy dependent spectra.

For comparison of spectra I propose that we use the TART definition to include all neutrons introduced into the system as production, and all neutrons that are absorbed or leaked as removal. In which case (n,2n), (n,3n), etc., make positive contributions to both production and removal. For our comparisons tally the following quantities at the energies at which the event happened, not the energy at which neutrons were subsequently re-emitted. For example, for fission tally one neutron removal and $< \nu >$

neutrons produced at the energy where the fission was induced, not the fission emission spectrum in which the neutrons are emitted; the former is very specific for each system and will provide us with the information that we need, the latter will not.

Production = $< \nu > \Sigma f + 2\Sigma n,2n + 3\Sigma n,3n + ...$
Absorption = $\Sigma n,0 + \Sigma f + \Sigma n,2n + \Sigma n,3n + ...$
Leakage = L

These quantities are integrated over the entire system, such that if we further integrate the spectra over energy we should be able to exactly reproduce K-eff,

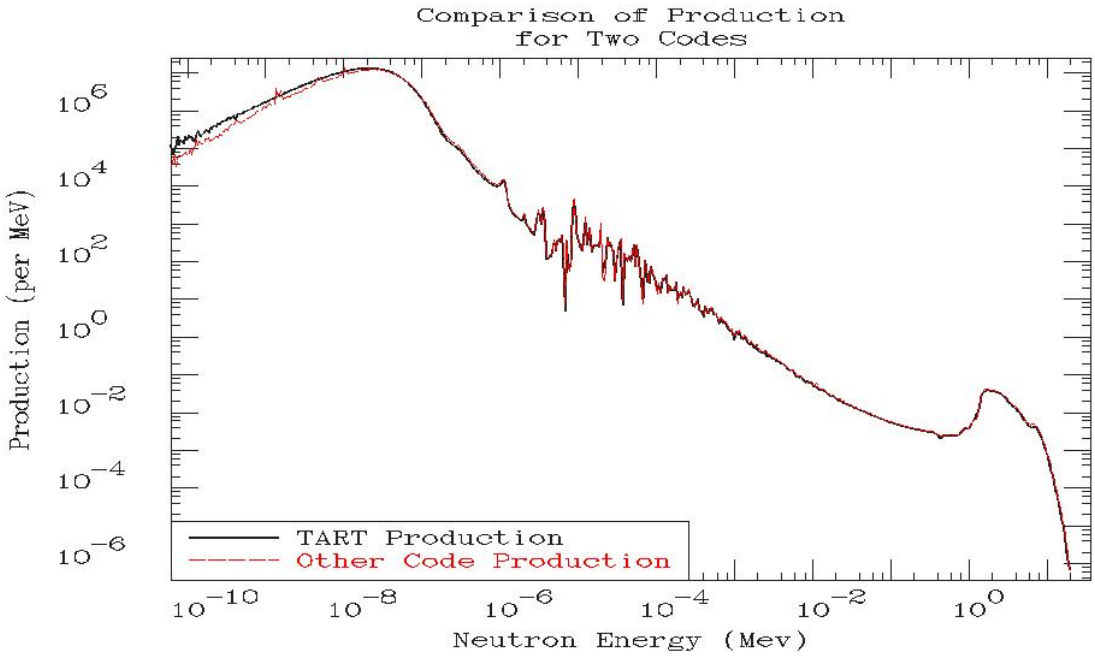
K-eff = [Production]/[Absorption + Leakage]

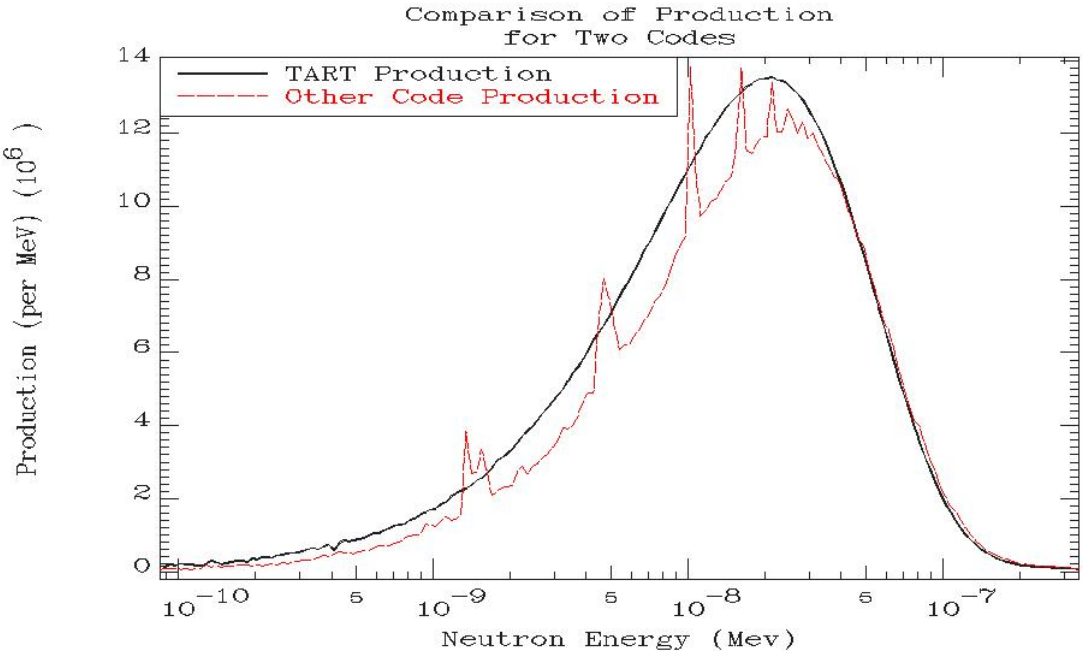
Tally from 10^{-11} MeV to 20 MeV using the TART 616 energy tally bin structure. The definition of the tally bin index is trivial, since there are 50 tally bins per energy decade, uniformly spaced in lethargy (log of energy),

Index = $0 < 10^{-11}$ MeV
= 1 to 616 : 10^{-11} MeV to 20 MeV = 1 + 50*alog10(E/10^{-11}); E in MeV
= 617 > 20 MeV

So that in the future we can compare code results in greater detail, if any code designer adds these quantities to the output of their code in any format that they want, I (Red Cullen) will ”volunteer” to write a utility code to put your results into a standard form for comparison to the detailed output from other codes. We already have a number of codes which are connected in this manner, and our results are providing a great deal of insight and understanding to the differences we see in the output from a variety of codes.

As an example of how much we can learn from detail comparisons, I selected two codes that produce very similar results for simple integral parameters such as K-eff for our pin cell problems. Below I show a detailed comparison of the neutron production spectra. In the first figure we can see excellent agreement over most of the energy range, except for at very low energy. The second figure shows a detail of the very low energy, and from this can can see that one code is modeling the thermal scattering law continuous in secondary energy, whereas the other is modeling it as a series of discrete secondary energies for hydrogen bound in water. The only reason that this second spectrum does not drop lower between the discrete energies, is because of free atom scattering in oxygen and to a lesser degree uranium.


Comparison of Production
for Two Codes
Production (per MeV)
TART Production
Other Code Production
Neutron Energy (Mev)


Comparison of Production
for Two Codes
Production (per MeV) (10^6)
TART Production
Other Code Production
Neutron Energy (Mev)

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